TM on Nuclear Data Retrieval, Dissemination, and Data Portals

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Book of Abstracts

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Nuclear data processing codes and steps - a primer

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Nuclear data processing systems need to be used to convert evaluations in the Evaluated Nuclear Data Files (ENDF-6) format into forms useful for practical applications. Each application, dedicated analysis, assessment that rely on nuclear data have specific, sometimes unique nuclear data form needs, requirements and priority. Nuclear data portals are no exception and require specific, dedicated forms to efficiently serve a diverse user's needs.

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TM on Nuclear Data Retrieval, Dissemination, and Data Portals

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"TM on Nuclear Data Retrieval, Dissemination, and Data Portals"aims to:
• Evaluate existing tools and their capabilities such as:
- Web-API's and other data retrieval methods
- GUI's
- Format conversion tools useful for the Data Portal development
• Review some use-cases,
• Discuss challenges in data format conversion and nuclear data pipelines
• Discuss best practises which would be necessary to establish an efficient Nuclear Data Portal

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Opening remarks and administrative matters

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Ideas on a decentralized, inclusive and traceable nuclear data future

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By framing problems with specific words, we also prime thought networks for determining possible solutions. The phrasing “data portal” is one such specific phrasing, “data networks” or “data flows” would be other choices inducing different thoughts. In this contribution, I want to take as starting point the idea of “data flows”. More specifically, several prominent nuclear data sources exist (e.g. EXFOR, evaluated nuclear data libraries, model codes), and irrespective of the use of the data, we can always say that the data flows from one or several sources to intermediate points, potentially merging with other data flows, before it ends up at some endpoint. During this process, the data may become filtered, enriched or transformed. These data flows, travelling through systems and directed by persons are quite opaque in the past and are still not easily traceable in the present. In this contribution, I want to present some perspectives and ideas on how we could make these data flows transparent, traceable and hence reproducible, potentially providing benefits to both established researchers in the nuclear data field and newcomers.

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Nuclear Data Service System of the China Nuclear Data Center（NDS-C）

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The China Nuclear Data Center attaches great importance to the processing and visualization of nuclear data, as well as providing online data services. After more than two decades of effort, it has developed its own online nuclear data service system, named as NDS-C. This system utilizes API technology to offer a unified data processing interface that can serve a variety of applications across different environments, thereby enhancing development efficiency and reducing the complexity of system maintenance. It achieves an all-in-one project file that includes graphic elements, data elements, and information elements, among others. The system is capable of processing evaluation data in the ENDF format, experimental data in the EXFOR format, free-form data, and graphical data. The EXFOR and ENDF data are efficiently converted into hierarchical structures, which simplifies the correlation between data and facilitates in-depth data processing and mining. The service supports the development of browsers, desktop systems, and mobile applications, catering to the diverse needs of various users for nuclear data. NDS-C has a broad user base in China, with applications ranging from nuclear facilities and engineering to nuclear instruments, nuclear fuel materials, scientific research, data evaluation, and nuclear reaction experiments. These users have a wide array of requirements. For those engaged in nuclear reaction experiments and nuclear engineering, functions for processing and analyzing data on natural nuclides have been integrated. For general scientific research users, a convenient mobile application featuring fission yield data and decay data has been provided. For users in the fields of nuclear reactors and nuclear chemistry, a more specialized desktop software incorporating these data has been developed. For nuclear data evaluators, a batch plotting system for the entire library evaluation has been established, along with features such as emitted particle energy spectrum shape analysis, covariance data analysis, curve summation, ratio analysis, and graphical digitization tools. Additionally, training datasets based on EXFOR experimental data of nuclear reaction cross-sections have been offered for machine learning purposes.

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Social dinner

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Developments of IAEA Nuclear Data Explorer: Experimental and Evaluated Nuclear Data Libraries Visualization and Retrieval System

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The utilization of experimental nuclear reaction data in the EXFOR format and evaluated nuclear data in the ENDF-6 format necessitates preprocessing, which remains challenging for users aiming to apply contemporary computational methods in their modern data analysis and nuclear data evaluation efforts.

To address this issue, the IAEA Nuclear Data Section is tasked with developing access to EXFOR and ENDF-6 data, such as the EXFOR and ENDF web retrieval systems. With the rapid advances in computing infrastructure and the increasing demand to process nuclear data at scale for ML and AI applications, additional flexible retrieval options and open-source programs distributed under a permissive license will be beneficial to the nuclear data community. This will facilitate interdisciplinary collaboration among researchers and scientists in the fields of nuclear physics, nuclear data, and nuclear applications.

To enhance the accessibility and openness of EXFOR datasets, both the data and related codes need to adhere to the requirements established in SG50. This includes (1) open-source EXFOR parsing software to convert the existing EXFOR format into a more computationally accessible format and (2) a web service that implements the FAIR principles (Findable, Accessible, Interoperable, Reusable).

To meet these requirements, we have developed EXFOR parsing computer programs (EXFOR Parser) in Python to convert data from the EXFOR format to JSON. These JSON files are further converted into tabulated (x, y) data and pre-processed evaluated nuclear data libraries. Additionally, we have developed the visualization web system, IAEA Nuclear Reaction Data Explorer, and its APIs. In this presentation, we will explain the current data models and pipeline, as well as the necessary further developments.

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Ideas and concept for nuclear data management - A brainstorming session on data portal building blocks

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Standardizing data and unifying data access in the nuclear field opens a new dimension of data usage, especially in the age of machine-learning. For the development of those standards and infrastructures we should build on existing tools and established standards and infrastructures as much as possible, exploiting implicit knowledge present in existing technologies.
This presentation demonstrates a non-exhaustive overview of existing tools and infrastructures of relevance for the development of a central data portal. It gives experience feedback where possible and provides a starting point for discussions on how such a system can be implemented.

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Nuclear Data Editing Functions of FRENDY

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This presentation explains the nuclear data editing and drawing functions of FRENDY. FRENDY has editing functions to modify nuclear data files and to confirm processing results. Though many nuclear data processing codes have such functions, they can not process the nuclear data, e.g., resonance reconstruction, linearization, and Doppler broadening. If users want to edit nuclear data files, they have to process them. FRENDY's function automatically processes the nuclear data before editing. It can also generate multi-group cross section files from pointwise data. This function makes it easy for anyone to edit and draw nuclear data files. This presentation also explains other useful functions in FRENDY, such as the NJOY input file generation function.

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The need for new EXFOR formats to apply machine learning techniques to its data

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Will follow.

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Challenges in unifying nuclear data access

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This presentation aims to open the discussion how scientific nuclear reaction data can be best be brought to the users.
As GUI's are no longer the only way to access data, a scheme for basic nuclear data retrieval needs to be set to allow both computational access, though web-api's or similar tools, to the data and plotting abilities.

While quite some progress has been made for nuclear structure (ENSDF) data (see other contributions to this meeting), the tools for arguably the most important reaction databases, EXFOR and ENDF, are not yet in a state of general access: the user is forced to understand the ENDF and EXFOR logic and to work through a variety of format and exception rules.
Some initiatives are halfway. Modest examples by the author given here are EXFORtables and ENDFtables, to represent experimental and evaluated nuclear reaction data respectively, both meant to represent very format and database specific data into easy accessible form for nuclear scientists
Other, more complete, tools by others for this are underway but still need to prove its success and comprehensiveness.

A relatively light unifying format called YANDF (Yet Another Nuclear Data Format) is proposed.
Several relevant nuclear databases require an update, both in completeness and in format unification.
Examples are thermal neutron cross sections, resonance integrals, resonance parameters, Maxwellian-averaged cross sections, average radiative widths, evaluated gamma activation data, etc. etc.
If these and the other abovementioned databases should ever make it to ML applications, rich metadata will be required.

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IAEA's Data Journey: Strategic Approaches, Governance, and Collaborative Operating Models

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The Agency's mandate relies heavily on data-driven initiatives, showcasing progress in specific domains. However, data management has historically been fragmented. This inconsistency has led to a disconnect between data investments and their impact on business outcomes, preventing the full harnessing of data assets.

A cohesive approach is needed to align data governance, privacy, and usage with measurable business outcomes. The data strategic roadmap includes an adaptive governance framework, hybrid operating models, and capabilities to address the entire data landscape, balancing innovation and responsibility while minimizing risks.

The Agency's data journey is moving from a fragmented approach to a cohesive strategy that enhances decision-making, unlocks insights, and aligns data initiatives with organizational objectives.

Goal 1: Data Use & Business Impact focuses on embedding data into decision-making, ensuring data is tied to business outcomes. This shift from reactive to proactive data usage aims to drive business outcomes.

Goal 2: Data Architecture & Governance emphasizes adaptive governance and the fusion of centralized and decentralized models. The focus is on robust frameworks that support innovation while maintaining compliance and control, balancing agility with governance.

Goal 3: Data Capabilities aims to enhance data maturity by fostering a data-driven culture. Building a data science ecosystem and promoting AI adoption are critical steps in evolving data literacy and innovation, embedding data into daily operations, and ensuring the Agency remains at the forefront of data-driven decision-making.

This transformative data journey has just begun under the initiative of the Chief Data Officer (CDO), in close collaboration with various departments and divisions, including the Nuclear Data Section, ensuring that all stakeholders are aligned and contributing to the Agency's unified data strategy.

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HEPData: repository for publication-related High-Energy Physics data

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HEPData (https://www.hepdata.net) is the primary open-access repository for publication-related tabular high-level data in the field of experimental particle physics, otherwise known as High-Energy Physics (HEP). It currently contains 138k data tables from more than 10k publications and it is widely used by the HEP community with 4.5 million page views in 2023. The HEPData project has a very long history extending over half a century back to the 1970s, with the data being migrated multiple times as databases and computing technology have evolved over the decades. The most recent redevelopment was undertaken in 2015/16 as a partnership between Durham University (UK) and CERN (Switzerland). This presentation will describe the technologies involved in the modern incarnation of HEPData and explain its operation and usage.

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API for ENSDF

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Data dissemination has moved from paper, to web pages, and recently to API retrieval. The presentation shows how the IAEA Nuclear Data Section has evolved its tools to facilitate this trend.

The example of data API to describe decay chains highlights that defining the underlying data model takes precedence over the choice of the format.

Tools to translate json, xml, sql, hdf5, … into each other are now a commodity, whilst flaws in the data model, that might restrict the usefulness of the data, will not find solution in any format

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Data related to muon nuclear capture

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Cosmic-ray muons are constantly bombarding us on the ground. When a negative muon comes to rest in matter, it is captured into an atomic orbit and, with a certain probability, is subsequently absorbed by the atomic nucleus via the weak interaction. This process is known as muon nuclear capture (μNC). In this process, most of the muon's rest energy is carried away by a muon neutrino and the remaining energy excites the residual nucleus. μNC can be regarded as one of the most naturally occurring nuclear reactions.
Since μNC occurs ubiquitously on Earth, it holds significant relevance for various applications. A notable application is evaluating the soft error rate in semiconductor devices induced by cosmic-ray muons. Charged particles emitted following μNC can generate electron-hole pairs in semiconductors, potentially altering stored data and causing single event upsets (SEUs). This risk is growing as semiconductor devices become smaller and operate at lower voltages, making them more susceptible to such soft errors. Other applications include geochronology using cosmogenic nuclides generated by cosmic-ray muons and, of course, evaluating activation levels in muon facilities, where μNC plays an important role.
Despite the increasing need for muon nuclear data, a dedicated database has yet to be developed. While some muon nuclear reaction data are included in conventional databases such as ENSDF, the way of inclusion is not standardized. To address this, we launched the Muon Nuclear Data (μND)

Project, which aims to develop a comprehensive database for muon nuclear reactions. This database will include not only experimental data on muon nuclear reactions but also evaluated and theoretical data.
In this presentation, we will discuss the μNC process, the potential applications of μND, and also recent progress related to the μND project.

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The NDS infrastructure for FAIR Data

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The Nuclear Data Section is undergoing significant modernization efforts to align with FAIR (Findable, Accessible, Interoperable, and Reusable) data principles. This presentation will talk about the development of a new NDS website, implementation of APIs for improved data access for some of our databases (Stopping Powers, IDB, PSF), integration of Digital Object Identifiers (DOI) for permanent data citation, and adoption of open data standards. The talk will highlight the technical architecture behind these changes and discuss their impact on data preservation and accessibility.

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ENSDF Modernization

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The National Nuclear Data Center (NNDC) at Brookhaven National Laboratory (BNL) has recently undertaken a significant modernization of the Evaluated Nuclear Structure Data File (ENSDF) format, transitioning from a legacy 80-column ASCII format to JSON. This new hierarchical JSON format leverages a modern format consisting of key-value pairs, enabling efficient data organization, flexibility, and optimal compatibility for web-based data dissemination. However, the shift to JSON requires substantial adaptation of the existing codebases, as much of the current nuclear data software ecosystem is deeply reliant on the fixed-width ASCII format. The transition involves updating numerous codes, tools, and workflows to align with the modernized JSON schema, presenting both challenges and opportunities for improved data handling.

To facilitate this modernization, the NNDC is developing the ENSDF Editor, software tailored for ENSDF evaluator evaluation efforts. This editor is designed to provide an integrated environment where evaluators can efficiently review, evaluate, and edit nuclear structure data in the new JSON format. Built using advanced technologies such as Electron, a framework that combines Chromium and Node.js, the ENSDF Editor aims to deliver a cross-platform desktop experience that ensures consistency, performance, and accessibility across various operating systems. This tool will be instrumental in supporting evaluators as they transition to the updated format, ultimately enhancing the accessibility and usability of nuclear data for research, development, and applications in the nuclear science community.

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From ENSDF to NuDat: Search, Filter and Visualize Nuclear Data

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The National Nuclear Data Center (NNDC) at Brookhaven National Laboratory (BNL) has developed NuDat, a powerful web application enabling users to explore comprehensive databases of nuclear structure, nuclear decay, and neutron-induced nuclear reaction data. As the primary interface for querying, visualizing, and disseminating data from the Evaluated Nuclear Structure Data File (ENSDF), NuDat provides access to authoritative evaluated nuclear structure and decay values derived from all published experimental data. Annually, NuDat supports over 7 million retrievals, serving a diverse audience in research, education, and various applied fields.

The technology behind NuDat, initially developed more than 15 years ago, has since been surpassed by significant advancements in web capabilities. The NNDC has modernized NuDat to deliver an enriched user experience that fosters both discovery and in-depth exploration of nuclear data properties. The updated NuDat incorporates HTML Canvas to create a dynamic and interactive chart of nuclides, allowing users to navigate a database of over 3,300 nuclides with fluid pan and zoom gestures. Additional features include customizable filters and data export options, which enhance usability and flexibility.

Further extending NuDat's capabilities, the NNDC is developing a 3D version of the application using Three.js. This 3D interface will enable users to explore the chart of nuclides in a fully immersive environment, complete with adjustable visualization settings, thereby offering a new dimension to the understanding of nuclear data. These advancements in NuDat underscore NNDC's commitment to providing cutting-edge tools for the nuclear science community and beyond.

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ENDF Landing Pages and DOI Efforts

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The National Nuclear Data Center (NNDC) at Brookhaven National Laboratory (BNL) has recently released ENDF/B-VIII.1, the latest version of the Evaluated Nuclear Data File (ENDF) library. Produced, distributed, and endorsed by the Cross Section Evaluation Working Group (CSEWG), ENDF/B-VIII.1 represents the most current and comprehensive evaluated nuclear data resource, designed for a wide range of nuclear science and technology applications. This release brings important updates to the data, enhancing its accuracy and applicability for both research and industry.

In conjunction with this new library, the NNDC has launched an updated version of the ENDF web interface in a soft release. This new interface provides users with a streamlined and modernized way to access and navigate ENDF resources. At its core is the ENDF releases landing page, a central hub that provides direct downloads for all ENDF versions. This page is built as a dynamic, data-driven web application, allowing users to seamlessly access different ENDF versions and sublibraries through user-friendly input controls and URL query parameters.

As part of ongoing efforts to enhance discoverability and scholarly accessibility, the NNDC is currently organizing metadata for ENDF/B-VIII.1 and prior versions to obtain Digital Object Identifiers (DOIs) through the BNL library system. These DOIs, once registered through the Department of Energy's Office of Scientific and Technical Information (OSTI) and DataCite, will facilitate citation,

tracking, and academic referencing of ENDF data, aligning it with modern standards of scientific data management and dissemination.

Users' Feedbacks and New Demands / 20

Some User' Feedbacks and Potential new Demands

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The aim of this presentation is to present a collection of personal - failure and success - feedbacks with different nuclear data tools and nuclear data management systems (NDMS). I hope, this will open the discussion to improve current NDMS and retrieval/visualization tools, and to identify potential new features to enhance the usage and the quality of these systems. Finally, a summary of dissemination/training activities with students and users will be presented within the UPM and the EU/ GreatPioneer project.

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The NJOY modernization and the use of data interfaces

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will follow

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Dissemination of the recommendations from the Decay Data Evaluation Project

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The Laboratoire National Henri Becquerel is the French national metrology laboratory for ionizing radiation, in charge of the definition of the derived SI units –the becquerel (activity) and the gray and sievert (absorbed dose and dose equivalent) and their transfer to users. In order to define the becquerel with high precision, decay data are of utmost importance and an accurate knowledge of the decay scheme is mandatory. As a consequence, the LNHB has been involved for more than 50 years in the evaluation, recommendation and the provision of decay data. In particular, the LNHB is currently in charge of the coordination of the international Decay Data Evaluation Project, which aims at providing decay data to non-specialists, especially within the metrology community for intercomparison exercises. In this presentation, we will introduce the DDEP collaboration, the associated decay data evaluation work, its dissemination and associated software tools.

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Atomic, Molecular and Plasma-Material Interaction Databases at the IAEA

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The Atomic and Molecular Data (AMD) Unit [1] operates within the Nuclear Data Section (NDS) of the International Atomic Energy Agency with the primary objective to establish and maintain internationally recommended numerical databases of fundamental atomic and molecular data for fusion energy research and other plasma science and technology applications.

The CollisionDB database [2] is an important resource for plasma modellers which contains 122,612 collision cross section and rate coefficient data sets. This FAIR-compliant service is based on a relational database backend with complete metadata and an online, browser-based search interface which allows for data visualization. All data are timestamped, can be deprecated (but not deleted) and are associated with full bibliographic information concerning their source.
The CollisionDB service also exposes an API and a Python library, PyCollisionDB [3], has been released to utilise the API in that language.

A new database of plasma-material interaction data is under development. pwiDB [4] contains data sets concerning the sputtering, retention, diffusion, solubility and permeation of fuel and other ions in fusion reactor materials. In addition to online searching and visualization, data and all necessary contextual metadata can be downloaded in JSON format.

The AMD Unit's databases adopt common standards for the description of units [5], atomic and molecular species, states [6] and processes [7], agreed through experts'meetings and consultancies.

[1] https://amdis.iaea.org/
[2] https://amdis.iaea.org/db/collisiondb/
[3] https://github.com/IAEA-NDS/pycollisiondb
[4] https://db-amdis.org/pwidb/
[5] https://github.com/xnx/pyqn
[6] https://github.com/xnx/pyvalem
[7] https://amdis.iaea.org/databases/processes/

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chatNSR: An AI-Enhanced Nuclear Science References Knowledge Base

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We will provide an update on nascent efforts to compile for Neutron Science References using Large Language Models.

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A brief update on x4i

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We provide an update on recent improvements to the EXFOR API, x4i.

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endf-parserpy: A Python package for working with ENDF-6 files

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The handling of ENDF-6 files is often perceived as cumbersome, especially regarding their creation. The Python package *endf-parserpy* has been created with the objective of providing a handy tool to facilitate the interaction with ENDF-6 files. This contribution will present design considerations and capabilities of this package.

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Berkeley Nuclear Database Projects: Neutron Capture

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Berkeley Nuclear Database Projects: Structure and Decay

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The "Baghdad Atlas"as a Validation Tool for Evaluated Nuclear Data Libraries

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An Update on the High Priority Nuclear Structure Request List Website

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NSR Modernization

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The National Nuclear Data Center (NNDC) at Brookhaven National Laboratory (BNL) maintains several databases dedicated to physics research. One of these is Nuclear Science References (NSR), a bibliographic database for tracking research articles. The NNDC provides access to NSR through a website of the same name. However, several aspects of NSR's design make it difficult to maintain. NSR entries are stored in an 80-column "exchange"text file format which requires custom parsing. This format also lacks space for adding further information (i.e. ORCID for authors). Lastly, NSR only exists as a MariaDB database with no mechanisms for version control or tracking changes.
The NNDC is addressing these issues by taking steps to modernize the NSR database. A JSON schema for NSR has been developed to provide its data in a standard, widely used format. This schema will have room for additional fields to enable updating older entries. A set of executable programs has also been written to standardize conversion from exchange files to JSON files. Finally, all of NSR's exchange and JSON files have been stored in a Git repository from which they can be tracked and shared among developers. These modernization efforts have already facilitated website updates and collaboration with other bibliographic databases. In future, they will also help make NSR easier to distribute and expand upon.

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NNDC Mobile Apps

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The National Nuclear Data Center (NNDC) at Brookhaven National Laboratory (BNL) maintains several websites for distributing data. While these are useful resources, accessing them requires an Internet connection which may not be available. To provide offline alternatives, the NNDC has developed mobile applications for use on smartphones. By installing these apps, users can bring NNDC data into locations without W-Fi coverage. And unlike simply giving users the relevant data, distributing these apps enables the NNDC to provide search capabilities through user interfaces. The NNDC has developed mobile apps for two data sets –the Nuclear Wallet Cards (ground- and isomer-states), and the CapGam collection (thermal neutron capture). The Android versions of these applications are already available through Google Play, while the iOS versions are designed to add further plotting functions. Changes to these datasets can also be distributed through releasing new versions with current data. By releasing these mobile apps, the NNDC aims to improve its services for smartphone users.